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TREND-FREE BLOCK DESIGNS: THEORY[1]

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A common polynomial trend in one or more dimensions is assumed to exist over the plots in each block of a classical experimental design. An analysis of covariance model is assumed with trend components represented through use of orthogonal polynomials. The objective is to construct new designs through the assignment of treatments to plots within blocks in such a way that sums of squares for treatments and blocks are calculated as though there were no trend and sums of squares for trend components and error are calculated easily. Such designs are called trend-free and a necessary and sufficient condition for a trend-free design is developed. It is shown that these designs satisfy optimality criteria among the class of connected designs with the same incidence matrix. The analysis of variance for trend-free designs is developed. The paper concludes with two examples of trend-free designs.

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1. Motivation, introduction and summary. Various experimental designs have been considered for the two-way elimination of heterogeneity, the latin square being the best known. Many experimental situations arise in which response may be affected by the spatial or temporal position of the experimental unit or plot within a block and, frequently, an assumption of a common polynomial trend of specified degree over plots within blocks may be appropriate. The $v \times v$ latin square may be used to eliminate the effects of a common, one-dimensional, polynomial trend to degree $v - 1$ over the plots in rows of the square. Questions of criteria for and the optimality of other block designs, complete or incomplete, that eliminate the effects of common polynomial trends of specified degree over the plots within blocks are investigated. Examination of the existence and construction of the desired designs is deferred to a subsequent paper.

Experimental designs to be used in the presence of trends to avoid the complications of analysis of covariance and to increase design efficiencies have been developed by others. Cox (1951, 1952, 1958) considered the assignment of treatments to plots ordered in space or time without blocking and with a trend extending over the entire sequence of plots. Box (1952) and Box and Hay (1953) in similar experimental sequences investigated choices of levels of quantitative factors. Hill (1960) combined the designs of Cox and Box to form new designs to study the effects of both qualitative and quantitative factors in the presence of trends. Daniel and Wilcoxon (1966) and Daniel (1976, Chap. 15) provided methods of sequencing the assignments of factorial treatment combinations to experimental units to achieve better estimation of specified factorial effects, again in the presence of a trend in time or distance. Phillips (1964, 1968a, 1968b) illustrated the use of magic figures (magic squares, magic rectangles, etc) for the elimination of trend effects in certain classes of one-way, factorial, latin-square, and graeco-latin-square designs; a single trend was assumed again to affect all of the observations.

We consider block designs to compare v treatments in b blocks of equal size $k \leq v$ such that each treatment occurs at most once in each block. A common polynomial trend is assumed to exist over the plots in each block. The trend may be in one or several dimensions and is expressed in terms of $p \leq (k - 1)$ orthogonal components. The appropriate classical fixed-effects model for the general block design and its assumptions are used with the addition of orthogonal terms representing the assumed trend. The problem is to assign treatments to plots within blocks so that the known properties of the ordinary analysis of variance for treatment and block sums of squares are preserved and variation due to the trend may be removed from the error sum of squares. When the desired designs exist, we shall call them trend-free designs. We shall abbreviate and, for example, use TF_pCB for a complete block design free of a common, one-dimensional trend of degree p within blocks and TF_pBIB and TF_pPBIB for similar balanced and partially balanced incomplete block designs. Additional subscripts may be added if the trend is in several dimensions.

In this paper, necessary and sufficient conditions for the existence of trend-free block (TFB) designs are obtained, necessary analysis of variance is developed, and optimality properties are demonstrated. Several examples of TFB designs are included but results on design construction are not included.

2. Notation, definitions and model. Let v treatments be applied to plots arranged in b blocks, each of size k, $k \leq v$. Each plot receives only one treatment and each treatment occurs at most once in a block. The plot positions

in a block are indexed by m-dimensional vectors of positive integers, $\underset{\sim}{t} = (t_1, \ldots, t_m)$, $t_u = 1, \ldots, s_u$, $u = 1, \ldots, m$, where s_u is the number of plot positions in the u-th dimension, $\prod_u s_u = k$. The polynomial trend extending over plots in each block is a function of the plot position $\underset{\sim}{t}$ and is expressed as a linear function of m-dimensional orthogonal polynomials of the form, $\phi_{\underset{\sim}{\alpha}}(\underset{\sim}{t}) \equiv \phi_{(\alpha_1,\ldots,\alpha_m)}(t_1, \ldots, t_m) = \prod_{u=1}^{m} \phi_{\alpha_u}(t_u)$, where $\phi_{\alpha_u}(t_u)$ is a one-dimensional orthogonal polynomial of degree α_u satisfying the orthogonality conditions, for $u = 1, \ldots, m$,

(2.1) $$\sum_{t_u=1}^{s_u} \phi_{\alpha_u}(t_u) = 0$$

and

(2.2) $$\sum_{t_u=1}^{s_u} \phi_{\alpha_u}(t_u)\, \phi_{\alpha'_u}(t_u) = \begin{cases} 1 & \text{if } \alpha_u = \alpha'_u, \\ 0 & \text{if } \alpha_u \neq \alpha'_u. \end{cases}$$

Note that multidimensional orthogonal polynomials may be obtained as indicated from one-dimensional ones and that $k = \prod_{u=1}^{m} s_u$. Tables of one-dimensional orthogonal polynomials for equally spaced variables are given by Fisher and Yates (1957).

The mathematical model is a simple extension of the classical model for general block designs, trend terms added, and is written

(2.3) $$y_{j\underset{\sim}{t}} = \mu + \sum_{i=1}^{v} \delta^{i}_{j\underset{\sim}{t}} \tau_i + \beta_j + \sum_{\underset{\sim}{\alpha}\in A} \theta_{\underset{\sim}{\alpha}}\, \phi_{\underset{\sim}{\alpha}}(\underset{\sim}{t}) + \varepsilon_{j\underset{\sim}{t}},$$

$$j = 1, \ldots, b,\ \underset{\sim}{t} = (t_1, \ldots, t_m),\ t_u = 1, \ldots, s_u,\ u = 1, \ldots, m,$$

where $y_{j\underset{\sim}{t}}$ is the observation on plot position $\underset{\sim}{t}$ of block j, μ, τ_i and β_j are respectively the usual mean, treatment and block parameters, A is an index set of p, m-dimensional, non-zero vectors of the form $\underset{\sim}{\alpha}$, and $\theta_{\underset{\sim}{\alpha}}$ is the regression coefficient of $\phi_{\underset{\sim}{\alpha}}(\underset{\sim}{t})$. The trend effect on plot position $\underset{\sim}{t}$ is $\sum_{\underset{\sim}{\alpha}\varepsilon A} \theta_{\underset{\sim}{\alpha}} \phi_{\underset{\sim}{\alpha}}(\underset{\sim}{t})$, not dependent on the particular block j. Designation of the treatment applied to plot (j, $\underset{\sim}{t}$) is effected through the indicator function,

$$(2.4) \qquad \delta^{i}_{j\underset{\sim}{t}} = \begin{cases} 1 & \text{if treatment } i \text{ on plot } (j, \underset{\sim}{t}), \\ 0 & \text{otherwise.} \end{cases}$$

The errors $\varepsilon_{j\underset{\sim}{t}}$ are assumed to be i.i.d. with zero means and they will be taken to be normal, $N(0, \sigma^2)$, in discussions of distribution theory below. The model (2.3) will be regarded as a fixed-effects model unless specifically stated to be otherwise in particular remarks.

Choices of values of $\delta^{i}_{j\underset{\sim}{t}}$ specify particular block designs. The construction of TFB designs is the determination of values of the $\delta^{i}_{j\underset{\sim}{t}}$ to meet criteria to be developed.

Some matrix notation will be needed. Let $\underset{\sim}{I}_n$ be the identity matrix of order n, $\underset{\sim}{0}_{m\times n}$ be the m × n null matrix, $\underset{\sim}{J}_{m\times n}$ be the m × n matrix with unit elements, $\underset{\sim}{1}_n$ be the n-dimensional column vector with unit elements, and $\underset{\sim}{B} \otimes \underset{\sim}{C}$, the Kronecker product of matrices $\underset{\sim}{B}$ and $\underset{\sim}{C}$. Lexicographic order is defined:

<u>Definition 2.1</u>. Two distinct vectors of non-negative integer elements, $\underset{\sim}{i} = (i_1, \ldots, i_m)$ and $\underset{\sim}{j} = (j_1, \ldots, j_m)$ are in lexicographic order if $\underset{\sim}{i}$ is ordered before $\underset{\sim}{j}$ whenever $i_1 = j_1, \ldots, i_{s-1} = j_{s-1}, i_s < j_s$ for some s, $1 \le s \le n$. Several distinct m-element vectors are in lexicographic order if all pairs of vectors are in lexicographic order.

The model (2.3) in matrix notation is

$$(2.5) \qquad \underset{\sim}{Y} = \underset{\sim}{X}\,\underset{\sim}{\gamma} + \underset{\sim}{E} = \underset{\sim}{X}_{\mu}\mu + \underset{\sim}{X}_{\tau}\underset{\sim}{\tau} + \underset{\sim}{X}_{\beta}\underset{\sim}{\beta} + \underset{\sim}{X}_{\theta}\underset{\sim}{\theta} + \underset{\sim}{E},$$

$\underset{\sim}{Y}$ and $\underset{\sim}{E}$ being bk-element column vectors with elements $y_{j\underset{\sim}{t}}$ and $\varepsilon_{j\underset{\sim}{t}}$ in subscript lexicographic order on $(j, \underset{\sim}{t})$, $\underset{\sim}{\tau}' = (\tau_1, \ldots, \tau_v)$, $\underset{\sim}{\beta}' = (\beta_1, \ldots, \beta_b)$, $\underset{\sim}{\theta}' = (\theta_{\underset{\sim}{\alpha}_1}, \ldots, \theta_{\underset{\sim}{\alpha}_p})$, $\underset{\sim}{\gamma}' = (\mu, \underset{\sim}{\tau}', \underset{\sim}{\beta}', \underset{\sim}{\theta}')$, $\underset{\sim}{X} = (\underset{\sim}{X}_\mu, \underset{\sim}{X}_\tau, \underset{\sim}{X}_\beta, \underset{\sim}{X}_\theta)$, $\underset{\sim}{X}_\mu = \underset{\sim}{1}_{bk}$, $\underset{\sim}{X}_\tau' = (\underset{\sim}{\Delta}_1', \ldots, \underset{\sim}{\Delta}_b')$, $\underset{\sim}{X}_\beta = \underset{\sim}{I}_b \otimes \underset{\sim}{1}_k$, $\underset{\sim}{X}_\theta = \underset{\sim}{1}_b \otimes \underset{\sim}{\phi}$, where $\underset{\sim}{\Delta}_j$ is the $k \times v$ matrix with $\delta^i_{j\underset{\sim}{t}}$ as the i-th element in row $\underset{\sim}{t}$ and $\underset{\sim}{\phi}$ is the $k \times p$ matrix with $\phi_{\underset{\sim}{\alpha}}(\underset{\sim}{t})$ in row $\underset{\sim}{t}$ and column $\underset{\sim}{\alpha}$, $\underset{\sim}{\alpha} \in A$, and the rows of $\underset{\sim}{\Delta}_j$ and $\underset{\sim}{\phi}$ being in subscript lexicographic order on $\underset{\sim}{t}$. For convenience, the vector-elements of $\underset{\sim}{\alpha}$ are taken also to be in lexicographic order. Conditions (2.1), (2.2) and (2.4) imply:

(2.6) $$\underset{\sim}{1}_k' \underset{\sim}{\phi} = \underset{\sim}{0}_{1\times p},$$

(2.7) $$\underset{\sim}{\phi}' \underset{\sim}{\phi} = \underset{\sim}{I}_p,$$

(2.8) $$\underset{\sim}{\Delta}_j \underset{\sim}{\Delta}_j' = \underset{\sim}{I}_k, \quad j = 1, \ldots, b.$$

Note that each $\underset{\sim}{\Delta}_j$ is a permutation matrix in view of (2.8) and the fact that all elements of $\underset{\sim}{\Delta}_j$ are 0 or 1.

Remark 2.1. It is necessary that $p < k$. From (2.7), since $\underset{\sim}{\phi}$ is $k \times p$, the rank of $\underset{\sim}{\phi}$ is p and it is necessary that $k \geq p$. If $k = p$, $\underset{\sim}{\phi}$ would be non-singular contradicted by (2.6). Hence $p < k$. The number of orthogonal polynomials defining the trend in (2.3) must be less than the number of plots per block.

3. A necessary and sufficient condition for a TFB design. The sums of squares for treatments (adjusted for blocks if necessary), blocks (unadjusted), and trend of the analysis of covariance for the design modelled by (2.5) or (2.3) are considered. The general approach of Searle (1975) is used. A design described by (2.5) is trend-free relative to the trend effects in that model

when the indicated treatment and block sums of squares may be calculated as though the trend effects were omitted from the model.

Some additional notation is needed. Let the reduction from the sum of squares $\underset{\sim}{Y}'\underset{\sim}{Y}$ to the appropriate residual sum of squares due to a fitting of the general linear model, $\underset{\sim}{Y} = \underset{\sim}{X}\underset{\sim}{\gamma} + \underset{\sim}{E}$, by least squares be denoted by $R(\underset{\sim}{\gamma})$. Given an appropriate partition of $\underset{\sim}{X}$ and $\underset{\sim}{\gamma}$, $\underset{\sim}{X} = (\underset{\sim}{X}_1, \underset{\sim}{X}_2)$ and $\underset{\sim}{\gamma}' = (\underset{\sim}{\gamma}_1', \underset{\sim}{\gamma}_2')$, the model becomes $\underset{\sim}{Y} = \underset{\sim}{X}_1\underset{\sim}{\gamma}_1 + \underset{\sim}{X}_2\underset{\sim}{\gamma}_2 + \underset{\sim}{E}$ and $R(\underset{\sim}{\gamma}) = R(\underset{\sim}{\gamma}_1, \underset{\sim}{\gamma}_2)$. Let

$$(3.1) \qquad R(\underset{\sim}{\gamma}_2|\underset{\sim}{\gamma}_1) = R(\underset{\sim}{\gamma}_1, \underset{\sim}{\gamma}_2) - R(\underset{\sim}{\gamma}_1)$$

represent the difference in reduction of sum of squares due to fittings of the models, $\underset{\sim}{Y} = \underset{\sim}{X}\underset{\sim}{\gamma} + \underset{\sim}{E}$ and $\underset{\sim}{Y} = \underset{\sim}{X}_1\underset{\sim}{\gamma}_1 + \underset{\sim}{E}$. In our problem, $R(\underset{\sim}{\tau}|\mu, \underset{\sim}{\beta}, \underset{\sim}{\theta})$ and $R(\underset{\sim}{\beta}|\mu, \underset{\sim}{\theta})$ represent the desired treatment and block sums of squares and $R(\underset{\sim}{\tau}|\mu, \underset{\sim}{\beta})$ and $R(\underset{\sim}{\beta}|\mu)$ represent the corresponding sums of squares for the model like (2.5) with trend effects deleted. The circumstances under which

$$(3.2) \qquad R(\underset{\sim}{\tau}|\mu, \underset{\sim}{\beta}, \underset{\sim}{\theta}) = R(\underset{\sim}{\tau}|\mu, \underset{\sim}{\beta})$$

and

$$(3.3) \qquad R(\underset{\sim}{\beta}|\mu, \underset{\sim}{\theta}) = R(\underset{\sim}{\beta}|\mu)$$

are investigated.

The sums of squares in (3.2) and (3.3) are obtained by the Searle method. We have

$$(3.4) \qquad R(\underset{\sim}{\tau}|\mu, \underset{\sim}{\beta}, \underset{\sim}{\theta}) = \underset{\sim}{Y}'\underset{\sim}{D}_1\underset{\sim}{X}_\tau\underset{\sim}{Q}_1^-\underset{\sim}{X}_\tau'\underset{\sim}{D}_1\underset{\sim}{Y},$$

$$(3.5) \qquad R(\underset{\sim}{\tau}|\mu, \underset{\sim}{\beta}) = \underset{\sim}{Y}'\underset{\sim}{D}_2\underset{\sim}{X}_\tau\underset{\sim}{Q}_2^-\underset{\sim}{X}_\tau'\underset{\sim}{D}_2\underset{\sim}{Y},$$

and

$$(3.6) \qquad R(\underset{\sim}{\beta}|\mu, \underset{\sim}{\theta}) = R(\underset{\sim}{\beta}|\mu) = \frac{1}{k}\underset{\sim}{Y}'\underset{\sim}{X}_\beta\underset{\sim}{X}_\beta'\underset{\sim}{Y} - \frac{1}{bk}(\underset{\sim}{X}_\mu'\underset{\sim}{Y})^2,$$

where

$$(3.7) \qquad \underset{\sim}{D}_i = \underset{\sim}{I}_{bk} - \underset{\sim}{X}_i(\underset{\sim}{X}_i'\underset{\sim}{X}_i)^-\underset{\sim}{X}_i',$$

and

$$(3.8) \qquad \underset{\sim}{Q}_i = \underset{\sim}{X}_\tau'\underset{\sim}{D}_i\underset{\sim}{X}_\tau, \; i = 1, 2,$$

$$(3.9) \qquad \underset{\sim}{X}_1 = (\underset{\sim}{X}_\mu, \underset{\sim}{X}_\beta, \underset{\sim}{X}_\theta), \; \underset{\sim}{X}_2 = (\underset{\sim}{X}_\mu, \underset{\sim}{X}_\beta)$$

and $\underset{\sim}{A}^-$ is a generalized inverse of a matrix $\underset{\sim}{A}$, $\underset{\sim}{A}\underset{\sim}{A}^-\underset{\sim}{A} = \underset{\sim}{A}$. It is obvious from (3.6) that the trend effects in the model (2.5) do not affect calculation of the unadjusted block sum of squares nor do the values of the $\delta^i_{j\underset{\sim}{t}}$ in $\underset{\sim}{\Delta}_j$. This is intuitively clear since trend effects have zero sums over plots within blocks from (2.1) and the definition of $\phi_{\underset{\sim}{\alpha}}(\underset{\sim}{t})$. The ordinary block sum of squares calculated from block totals results from (3.6). But (3.4) and (3.5) depend on $\underset{\sim}{X}_\tau$ and hence may depend on the $\delta^i_{j\underset{\sim}{t}}$ when the model (2.5) applies. We show that (3.5) does not depend on choices of the $\delta^i_{j\underset{\sim}{t}}$, give a definition for the trend-free concept, and develop a necessary and sufficient condition for a design to be trend free.

Consider $\underset{\sim}{X}_i(\underset{\sim}{X}_i'\underset{\sim}{X}_i)^-\underset{\sim}{X}_i'$, i = 1, 2, in (3.7). Searle (1971, p. 20) shows that this quantity is invariant to the choice of the generalized inverse and it may be verified that we may take

$$(3.10) \qquad (\underset{\sim}{X}_1'\underset{\sim}{X}_1)^- = \begin{bmatrix} 0 & \underset{\sim}{0} & \underset{\sim}{0} \\ \underset{\sim}{0} & \frac{1}{k}\underset{\sim}{I}_b & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{0} & \frac{1}{b}\underset{\sim}{I}_p \end{bmatrix} \text{ and } (\underset{\sim}{X}_2'\underset{\sim}{X}_2)^- = \begin{bmatrix} 0 & \underset{\sim}{0} \\ \underset{\sim}{0} & \frac{1}{k}\underset{\sim}{I}_b \end{bmatrix}.$$

Then

$$D_1 = I_{bk} - \frac{1}{k} X_\beta X_\beta' - \frac{1}{b} X_\theta X_\theta'$$

(3.11) and

$$D_2 = I_{bk} - \frac{1}{k} X_\beta X_\beta'.$$

Since $X_\tau' X_\tau = D_R$, the diagonal matrix with i-th diagonal element r_i, the number of replications of treatment i, and $X_\tau' X_\beta = N$, the $v \times b$ incidence matrix with elements n_{ij}, $n_{ij} = 1, 0$, as treatment i is, is not, in block j, Q_2 and Q_2^- do not depend on the δ_{jt}^i. Since $X_\tau' Y = T$, the column vector of treatment totals and $X_\tau' X_\mu = R$, the column vector with i-th element r_i, $X_\tau' D_2 Y$ does not depend on the δ_{jt}^i nor does (3.5). Thus (3.5) depends only on the usual observation totals and design parameters and is the usual treatment sum of squares for the block design calculated in the absence of trend terms in the model (2.5).

We continue with an explicit definition and a theorem.

Definition 3.1. A block design modelled by (2.5) is trend-free relative to the trend in the model if $R(\tau|\mu, \beta, \theta) = R(\tau|\mu, \beta)$.

Theorem 3.1. A necessary and sufficient condition for a block design to be trend-free is that

$$X_\tau' X_\theta = 0. \quad (3.12)$$

Proof. To prove necessity, equate (3.4) and (3.5), substitute from (3.7) and (3.8), and obtain the equality,

$$D_1 X_\tau Q_1^- X_\tau' D_1 = D_2 X_\tau Q_2^- X_\tau' D_2. \quad (3.13)$$

Pre- and post-multiplication of both sides of (3.13) by X'_τ and X_τ respectively reduce the equality to $Q_1 = Q_2$ or, equivalently, to

$$X'_\tau (D_2 - D_1) X_\tau = 0. \tag{3.14}$$

Use of (3.11) in (3.14) yields (3.12) to complete the proof of necessity.

To prove sufficiency, (3.12) is used with (3.11) to show that $Q_1 = Q_2$ and that $X'_\tau D_1 = X'_\tau D_2$ and the equality of (3.4) and (3.5) follows.

<u>Remark 3.1</u>. The design construction problem may be reformulated. Note that $X'_\tau = (\Delta'_1, \ldots, \Delta'_b)$, where each Δ_j is a permutation matrix. Then (3.12) is equivalent to

$$\sum_j \Delta'_j \phi = \Delta'_+ \phi = 0, \tag{3.15}$$

where $\Delta_+ = \sum_j \Delta_j$. The matrix Δ_+ has non-negative integer elements such that all row sums are b and column sums are r_i, $i = 1, \ldots, v$. The TFB design is constructed if Δ_+ satisfying (3.15) is found first and then if b permutation matrices Δ_j are found such that $\sum_j \Delta_j = \Delta_+$.

Notice that (3.15) implies that

$$\sum_{j=1}^{b} \sum_{t_1=1}^{s_1} \cdots \sum_{t_m=1}^{s_m} \delta^i_{jt} \, \phi_\alpha(t) = 0, \tag{3.16}$$

for all $i = 1, \ldots, v$ and all $\alpha \in \mathcal{A}$. In a TFB design, the total effect of each trend component over the plots assigned to any treatment is zero.

4. <u>Optimality properties of TFB designs</u>. Let us suppose that the primary purpose of an experiment is to compare treatment effects. Then it is desirable in most experiments that the treatment design matrix X_τ be chosen such that each

possible treatment difference, $\tau_i - \tau_{i'}$, $i \neq i'$, $i, i' = 1, \ldots, v$, be estimable under model (2.5) as stated or with trend components omitted. Designs with such a property have been defined to be connected. The selection of $\underset{\sim}{X}_\tau$ may be viewed as a two-stage process. The first stage is the determination of a way of blocking specified by the incidence matrix $\underset{\sim}{N} = \underset{\sim}{X}'_\tau \underset{\sim}{X}_\beta$ and the second stage is the allocation of treatments to plots within blocks. In this section we decompose the class of connected designs into subclasses with identical incidence matrices. Given (2.5), optimality properties possessed by TFB designs within these subclasses are considered.

The following familiar optimality definitions are considered over the subclass of connected designs under model (2.5) with the same incidence matrix:

(i) A design is $\bar{V}$-optimal if the average variance of the estimators of all elementary treatment contrasts, $\tau_i - \tau_{i'}$, is minimum.

(ii) A design is A-optimal if the trace of the covariance matrix of the estimators of any $v - 1$ orthonormal treatment contrasts is minimum.

(iii) A design is D-optimal if the determinant of the covariance matrix of (ii) is minimum.

(iv) A design is E-optimal if the largest eigenvalue of the covariance matrix of (ii) is minimum.

4.1. Estimability and connectedness. Consider the model (2.5), first in its general form, and a given non-null column vector $\underset{\sim}{u}$ of constants with proper dimension. It is well known that the definition of estimability implies that $\underset{\sim}{u}'\underset{\sim}{\gamma}$ is estimable if and only if

$$\text{rk}(\underset{\sim}{u}, \underset{\sim}{X}'\underset{\sim}{X}) = \text{rk}(\underset{\sim}{X}'\underset{\sim}{X}). \tag{4.1}$$

We use (4.1) with proper selection of $\underset{\sim}{u}$ to determine a necessary and sufficient condition for the estimability of a linear function of treatment parameters and consequently for the connectedness of a design.

The least-squares normal equation associated with (2.5) is $\underset{\sim}{X}'\underset{\sim}{X}\hat{\underset{\sim}{\gamma}} = \underset{\sim}{X}'\underset{\sim}{Y}$, where $\hat{\underset{\sim}{\gamma}}$ is the estimator of $\underset{\sim}{\gamma}$. Since $\underset{\sim}{N}'\underset{\sim}{1}_v = k\underset{\sim}{1}_b$, $\underset{\sim}{N}\underset{\sim}{1}_b = \underset{\sim}{R}$, and $\underset{\sim}{1}_v'\underset{\sim}{X}_\tau'\underset{\sim}{X}_\theta = \underset{\sim}{1}_{bk}'\underset{\sim}{X}_\theta = \underset{\sim}{0}_{1\times p}$, it reduces to

$$(4.2)\qquad \begin{bmatrix} bk & \underset{\sim}{R}' & k\underset{\sim}{1}_b' & \underset{\sim}{0}_{1\times p} \\ \underset{\sim}{R} & \underset{\sim}{D}_R & \underset{\sim}{N} & \underset{\sim}{X}_\tau'\underset{\sim}{X}_\theta \\ k\underset{\sim}{1}_b & \underset{\sim}{N}' & k\underset{\sim}{I}_b & \underset{\sim}{0}_{b\times p} \\ \underset{\sim}{0}_{p\times 1} & \underset{\sim}{X}_\theta'\underset{\sim}{X}_\tau & \underset{\sim}{0}_{p\times b} & b\underset{\sim}{I}_p \end{bmatrix} \begin{bmatrix} \hat{\mu} \\ \hat{\underset{\sim}{\tau}} \\ \hat{\underset{\sim}{\beta}} \\ \hat{\underset{\sim}{\theta}} \end{bmatrix} = \begin{bmatrix} G \\ \underset{\sim}{T} \\ \underset{\sim}{B} \\ \underset{\sim}{W} \end{bmatrix},$$

where $G = \underset{\sim}{X}_\mu'\underset{\sim}{Y}$, $\underset{\sim}{T} = \underset{\sim}{X}_\tau'\underset{\sim}{Y}$, $\underset{\sim}{B} = \underset{\sim}{X}_\beta'\underset{\sim}{Y}$, and $\underset{\sim}{W} = \underset{\sim}{X}_\theta'\underset{\sim}{Y}$, are the observation total and vectors of treatment, block and trend totals respectively. Let

$$(4.3)\qquad \underset{\sim}{H} = (\underset{\sim}{0}_{v\times 1}, \underset{\sim}{I}_v, -\frac{1}{k}\underset{\sim}{N}, -\frac{1}{b}\underset{\sim}{X}_\tau'\underset{\sim}{X}_\theta),$$

premultiply both sides of (4.2) by $\underset{\sim}{H}$, and obtain the reduced normal equation,

$$(4.4)\qquad \underset{\sim}{C}\hat{\underset{\sim}{\tau}} = \underset{\sim}{Q},$$

for the estimation of treatment parameters, where

$$(4.5)\qquad \underset{\sim}{C} = \underset{\sim}{D}_R - \frac{1}{k}\underset{\sim}{N}\underset{\sim}{N}' - \frac{1}{b}\underset{\sim}{X}_\tau'\underset{\sim}{X}_\theta\underset{\sim}{X}_\theta'\underset{\sim}{X}_\tau$$

and

$$(4.6)\qquad \underset{\sim}{Q} = \underset{\sim}{H}\underset{\sim}{X}'\underset{\sim}{Y} = \underset{\sim}{T} - \frac{1}{k}\underset{\sim}{N}\underset{\sim}{B} - \frac{1}{b}\underset{\sim}{X}_\tau'\underset{\sim}{X}_\theta\underset{\sim}{W}.$$

The matrix $\underset{\sim}{C}$ in (4.4) plays a decisive role in the estimation of a linear function of the treatment parameters and in the connectedness of a design under model (2.5). A linear function $\underset{\sim}{a}'\underset{\sim}{\tau}$ may be represented by $\underset{\sim}{u}'\underset{\sim}{\gamma}$ with

$$\underset{\sim}{u}' = (0, \underset{\sim}{a}', \underset{\sim}{0}_{1\times b}, \underset{\sim}{0}_{1\times p}), \tag{4.7}$$

$\underset{\sim}{a}$ being a ν-element column vector of constants. It may be shown that

$$\mathrm{rk}(\underset{\sim}{u}, \underset{\sim}{X}'\underset{\sim}{X}) = b + p + \mathrm{rk}(\underset{\sim}{a}, \underset{\sim}{C}) \tag{4.8}$$

by an argument similar to that of Chakrabarti (1962) for a model like (2.5) with trend effects absent. If $\underset{\sim}{a} = \underset{\sim}{0}_{\nu\times 1}$,

$$\mathrm{rk}(\underset{\sim}{X}'\underset{\sim}{X}) = b + p + \mathrm{rk}\underset{\sim}{C}. \tag{4.9}$$

Use of (4.8) and (4.9) in (4.1) demonstrates that a necessary and sufficient condition for the estimability of $\underset{\sim}{a}'\underset{\sim}{\tau}$ is that

$$\mathrm{rk}(\underset{\sim}{a}, \underset{\sim}{C}) = \mathrm{rk}\underset{\sim}{C}. \tag{4.10}$$

It follows further, through use of (4.10) and the argument by Raghavarao (1971, Theorem 4.2.2), that a design represented by (2.5) is connected if and only if $\mathrm{rk}\underset{\sim}{C} = \nu - 1$. For a TFB design $\underset{\sim}{C}$ reduces to $\underset{\sim}{C}_0 = \underset{\sim}{D}_R - \frac{1}{k}\underset{\sim}{N}\underset{\sim}{N}'$. We summarize our results:

<u>Theorem 4.1</u>. A TFB design under model (2.5) is connected if and only if $\mathrm{rk}(\underset{\sim}{D}_R - \frac{1}{k}\underset{\sim}{N}\underset{\sim}{N}') = \nu - 1$. If a TFB design exists, imposed on a connected block design with a model like (2.5) with trend effects absent, the TFB design is connected under (2.5).

4.2. Optimality properties. The main theorem on optimality follows:

Theorem 4.2. If a TFB design exists in a subclass of connected designs with a given incidence matrix, the TFB design is $\bar{V}$-, A-, D-, and E-optimal over the subclass.

To prove Theorem 4.2, some preliminary results, definitions, and lemmas are required.

It can be shown from (4.5) and (4.6) that

$$E(\underset{\sim}{Q}) = \underset{\sim}{C}\underset{\sim}{\tau} \text{ and } Var(\underset{\sim}{Q}) = \sigma^2\underset{\sim}{C}. \tag{4.11}$$

If $\underset{\sim}{a}'\underset{\sim}{\tau}$ is estimable, it is uniquely estimated by $\underset{\sim}{a}'\hat{\underset{\sim}{\tau}}$ and hence

$$E(\underset{\sim}{a}'\hat{\underset{\sim}{\tau}}) = \underset{\sim}{a}'\underset{\sim}{\tau} \text{ and } Var(\underset{\sim}{a}'\hat{\underset{\sim}{\tau}}) = \sigma^2\underset{\sim}{a}'\underset{\sim}{C}^+\underset{\sim}{a}, \tag{4.12}$$

where $\underset{\sim}{C}^+$ represents the Moore-Penrose inverse of $\underset{\sim}{C}$.

If any two square matrices $\underset{\sim}{A}$ and $\underset{\sim}{B}$ of the same order are considered, we define $\underset{\sim}{A} \geq \underset{\sim}{B}$ to mean that $\underset{\sim}{A} - \underset{\sim}{B}$ is positive semidefinite. Evidently, $\underset{\sim}{A} \geq \underset{\sim}{0}$ means that $\underset{\sim}{A}$ is positive semidefinite. Let the trace, determinant and largest eigenvalue of $\underset{\sim}{A}$ be tr$\underset{\sim}{A}$, $|\underset{\sim}{A}|$, and $\lambda_M(\underset{\sim}{A})$ respectively. The following lemmas assist in proof of Theorem 4.2.

Lemma 4.1. [Milliken and Akdeniz (1977)]. If $\underset{\sim}{A}$ and $\underset{\sim}{B}$ are two symmetric matrices of the same order and $\underset{\sim}{A} \geq \underset{\sim}{B} \geq \underset{\sim}{0}$, then $\underset{\sim}{B}^+ \geq \underset{\sim}{A}^+$ if and only if rk$(\underset{\sim}{A})$ = rk$(\underset{\sim}{B})$.

Lemma 4.2. For any two symmetric, positive semidefinite matrices $\underset{\sim}{A}$ and $\underset{\sim}{B}$ of the same order v and the same rank n, if $\underset{\sim}{A} \geq \underset{\sim}{B}$, then

(i) tr$(\underset{\sim}{B}^+) \geq$ tr$(\underset{\sim}{A}^+)$,

(ii) $|\underset{\sim}{K}\underset{\sim}{B}^+\underset{\sim}{K}'| \geq |\underset{\sim}{K}\underset{\sim}{A}^+\underset{\sim}{K}'|$,

(iii) $\lambda_M(\underset{\sim}{B}^+) \geq \lambda_M(\underset{\sim}{A}^+)$ and $\lambda_M(\underset{\sim}{K}\underset{\sim}{B}^+\underset{\sim}{K}') \geq \lambda_M(\underset{\sim}{K}\underset{\sim}{A}^+\underset{\sim}{K}')$, where $\underset{\sim}{K}$ is any $n \times v$ matrix such that $\underset{\sim}{K}\underset{\sim}{A}^{+}\underset{\sim}{K}'$ is positive definite.

Proof. Lemma 4.1 implies that $\underset{\sim}{B}^{+} \geq \underset{\sim}{A}^{+}$ and hence $\underset{\sim}{K}\underset{\sim}{B}^{+}\underset{\sim}{K}' \geq \underset{\sim}{K}\underset{\sim}{A}^{+}\underset{\sim}{K}'$. The proof of (i) is a consequence of the fact that each diagonal element of $\underset{\sim}{B}^{+}$ is not less than the corresponding one of $\underset{\sim}{A}^{+}$. The proof of (ii) follows from Rao (1973, p. 70). The proof of (iii) follows from the fact, given by Rao (1973, p. 62), that, for any symmetric matrix $\underset{\sim}{H}$,

$$\lambda_M(\underset{\sim}{H}) = \sup_{\underset{\sim}{x}} \frac{\underset{\sim}{x}'\underset{\sim}{H}\underset{\sim}{x}}{\underset{\sim}{x}'\underset{\sim}{x}}$$

where $\underset{\sim}{x}$ is any non-null column vector of proper dimension.

Lemma 4.3. If $\underset{\sim}{A}$ is a symmetric, positive semidefinite matrix of order v, then $n\,\mathrm{tr}(\underset{\sim}{M}) - \underset{\sim}{1}_n'\underset{\sim}{M}\underset{\sim}{1}_n \geq 0$ for any n-square principal minor $\underset{\sim}{M}$ of $\underset{\sim}{A}$.

Proof. Since $\underset{\sim}{A}$ is symmetric, positive semidefinite, so is $\underset{\sim}{M}$. Hence $\underset{\sim}{M}$ may be a covariance matrix of an $n \times 1$ random vector, say $\underset{\sim}{x}$. Let $\underset{\sim}{x}' = (x_1, \ldots, x_n)$ and $\underset{\sim}{M} = (m_{ij})$. The lemma follows from the fact that the average variance of all $x_i - x_j$, $i < j$, $i, j = 1, \ldots, n$, $\frac{2}{n(n-1)}[n\,\mathrm{tr}\underset{\sim}{M} - \underset{\sim}{1}_n'\underset{\sim}{M}\underset{\sim}{1}_n]$, is nonnegative.

We may proceed to the proof of Theorem 4.2.

Proof of Theorem 4.2. For a connected design, every elementary treatment contrast, $\tau_i - \tau_{i'}$, $i < i'$, $i, i' = 1, \ldots, v$, is estimable. From (4.12), we see that

$$\mathrm{Var}(\hat{\tau}_i - \hat{\tau}_{i'}) = (c^{ii} + c^{i'i'} - 2c^{ii'})\,\sigma^2,$$

where $c^{ii'}$, $i, i' = 1, \ldots, v$, is the (i, i')-element of $\underset{\sim}{C}^{+}$. Hence, the average variance $\bar{V}$ of the estimators of all elementary treatment contrasts is

$$\bar{V} = \frac{1}{\binom{v}{2}} \sum_{i=1}^{v} \sum_{\substack{i'=1 \\ i<i'}}^{v} \mathrm{Var}(\hat{\tau}_i - \hat{\tau}_{i'})$$

$$(4.13) \qquad = \frac{2\sigma^2}{v(v-1)} \sum_{i=1}^{v-1} \sum_{i'=i+1}^{v} (c^{ii} + c^{i'i'} - 2c^{ii'})$$

$$= \frac{2\sigma^2}{v(v-1)} [v \, \mathrm{tr}(\underset{\sim}{C}^+) - \underset{\sim}{1}_v' \underset{\sim}{C}^+ \underset{\sim}{1}_v].$$

We compare the general matrix $\underset{\sim}{C}$ with $\underset{\sim}{C}_0$ for the TFB design in the subclass of block designs with common incidence matrix $\underset{\sim}{N}$ and an existing TFB design:

$$\underset{\sim}{C}_0 - \underset{\sim}{C} = \frac{1}{b} \underset{\sim}{X}_\tau' \underset{\sim}{X}_0 \underset{\sim}{X}_0' \underset{\sim}{X}_\tau \geq \underset{\sim}{0}.$$

It follows from Lemma 4.1 that $\underset{\sim}{C}^+ - \underset{\sim}{C}_0^+ \geq \underset{\sim}{0}$ and hence

$$(4.14) \qquad v \, \mathrm{tr}(\underset{\sim}{C}^+ - \underset{\sim}{C}_0^+) - \underset{\sim}{1}_v'(\underset{\sim}{C}^+ - \underset{\sim}{C}_0^+)\underset{\sim}{1}_v \geq 0$$

by Lemma 4.3. Applying (4.13) to $\underset{\sim}{C}$ and $\underset{\sim}{C}_0$, and using (4.14), we have

$$\frac{2\sigma^2}{v(v-1)}[v \, \mathrm{tr}(\underset{\sim}{C}^+) - \underset{\sim}{1}_v' \underset{\sim}{C}^+ \underset{\sim}{1}_v] - \frac{2\sigma^2}{v(v-1)}[v \, \mathrm{tr}(\underset{\sim}{C}_0^+) - \underset{\sim}{1}_v' \underset{\sim}{C}_0^+ \underset{\sim}{1}_v] \geq 0,$$

which proves $\bar{V}$-optimality.

Let $\underset{\sim}{\Gamma}$ be any $(v - 1) \times v$ matrix such that $\underset{\sim}{\Gamma}\underset{\sim}{\Gamma}' = \underset{\sim}{I}_{v-1}$ and $\underset{\sim}{\Gamma}\underset{\sim}{1}_v = \underset{\sim}{0}_{(v-1)\times 1}$. Then $\underset{\sim}{\Gamma}\underset{\sim}{\tau}$ is a vector of $v - 1$ orthonormal treatment contrasts and $\mathrm{Var}(\underset{\sim}{\Gamma}\hat{\underset{\sim}{\tau}}) = \sigma^2 \underset{\sim}{\Gamma}\underset{\sim}{C}^+\underset{\sim}{\Gamma}'$. Since $\underset{\sim}{C}^+ \geq \underset{\sim}{C}_0^+$ and $\underset{\sim}{\Gamma}\underset{\sim}{C}^+\underset{\sim}{\Gamma}' \geq \underset{\sim}{\Gamma}\underset{\sim}{C}_0^+\underset{\sim}{\Gamma}'$, A-, D-, and E-optimality of the TFB design follow from (i), (ii), and (iii) respectively of Lemma 4.2.

The practical effect of Theorem 4.2 is to assure the user of TFB designs that they will be optimal as indicated relative to model (2.5) in comparison with the analysis of variance for the corresponding block design with treatments randomized over plots within blocks. The user of the TFB designs benefits also from the simpler available analysis of variance calculations.

5. Analysis of variance of TFB designs. Calculations and justifications for the analysis of variance of TFB designs may be developed by standard methods. A TFB design is derived from a standard block design for which the model is $\underset{\sim}{Y} = \underset{\sim}{X}_{\mu}\mu + \underset{\sim}{X}_{\beta}\underset{\sim}{\beta} + \underset{\sim}{X}_{\tau}\underset{\sim}{\tau} + \underset{\sim}{E}$, model (2.5) with trend terms deleted, and an analysis of variance table is available. That standard analysis of variance is used to obtain sums of squares for treatments (adjusted for blocks if necessary) and blocks (unadjusted) and the corrected total sum of squares for the analysis of variance of the TFB design with model (2.5). The sum of squares for trend with p degrees of freedom, when model (2.5) applies, is $\underset{\sim}{W}'\underset{\sim}{W}/b$, $\underset{\sim}{W} = \underset{\sim}{X}_{\theta}'\underset{\sim}{Y}$. The error sum of squares is obtained by subtraction. The sum of squares for trend is partitioned easily into components, W_i^2/b, $i = 1, \ldots, p$, each with one degree of freedom.

While the paragraph above describes the necessary calculations, the general analysis of variance for a TFB design is displayed in Table 1. In that table, G, $\underset{\sim}{T}$ and $\underset{\sim}{B}$ are as defined for (4.2) and

$$F = \frac{1}{k}\underset{\sim}{Y}'\underset{\sim}{X}'(\underset{\sim}{X}_{\beta}\underset{\sim}{X}_{\beta}' - \frac{1}{b}\underset{\sim}{X}_{\mu}\underset{\sim}{X}_{\mu}')\underset{\sim}{X}\underset{\sim}{Y}, \quad \underset{\sim}{C}_0 = \underset{\sim}{D}_R - \frac{1}{k}\underset{\sim}{N}\underset{\sim}{N}'.$$

The sums of squares are independent and, when divided by σ^2, have chi-square distributions with degrees of freedom (d.f.) given in Table 1 and non-centrality parameters obtainable from the expected mean squares of the table, expected mean square divided by σ^2 less one.

Table 1 is simplified in well known simple situations. For a TFCB design, $k = v$ and $r_i = b$, $i = 1, \ldots, v$, and then

$$F = v\underset{\sim}{\beta}'(\underset{\sim}{I}_b - \frac{1}{b}\underset{\sim}{1}_b\underset{\sim}{1}_b')\underset{\sim}{\beta}, \quad \underset{\sim}{C}_0 = b(\underset{\sim}{I}_v - \frac{1}{v}\underset{\sim}{1}_v\underset{\sim}{1}_v'),$$

$$\underset{\sim}{Q}'\underset{\sim}{C}_0^-\underset{\sim}{Q} = \frac{1}{b}(\underset{\sim}{T}'\underset{\sim}{T} - \frac{1}{v}G^2), \quad \underset{\sim}{\tau}'\underset{\sim}{C}_0\underset{\sim}{\tau} = b\underset{\sim}{\tau}'(\underset{\sim}{I}_v - \frac{1}{v}\underset{\sim}{1}_v\underset{\sim}{1}_v')\underset{\sim}{\tau},$$

and $\text{rk}\ \underset{\sim}{C}_0 = v - 1$.

For a TFBIB design with parameters v, b, k, r and λ,

$$\underset{\sim}{C}_0 = \frac{\lambda v}{k}(\underset{\sim}{I}_v - \frac{1}{v}\underset{\sim}{1}_v\underset{\sim}{1}_v'), \quad \underset{\sim}{Q}'\underset{\sim}{C}_0^-\underset{\sim}{Q} = \frac{k}{\lambda v}\underset{\sim}{Q}'\underset{\sim}{Q},$$

$$\underset{\sim}{\tau}'\underset{\sim}{C}_0\underset{\sim}{\tau} = \frac{\lambda v}{k}\underset{\sim}{\tau}'(\underset{\sim}{I}_v - \frac{1}{v}\underset{\sim}{1}_v\underset{\sim}{1}_v')\underset{\sim}{\tau}, \quad \text{and } rk\underset{\sim}{C}_0 = v - 1.$$

TABLE 1

General Analysis of Variance for a TFB Design, Model (2.5)

Source of Variation	d.f.	Sum of Squares	Expected Mean Square
Blocks (unadjusted)	b-1	$(\underset{\sim}{B}'\underset{\sim}{B}-\frac{1}{b}G^2)/k$	$\sigma^2+F/(b-1)$
Treatments (adjusted)	$rk\underset{\sim}{C}_0$	$\underset{\sim}{Q}'\underset{\sim}{C}_0^-\underset{\sim}{Q}$	$\sigma^2+(\underset{\sim}{\tau}'\underset{\sim}{C}_0\underset{\sim}{\tau})/rk\underset{\sim}{C}_0$
Trend Term 1	1	W_1^2/b	$\sigma^2+b\theta_1^2$
...	...	...	...
Trend Term p	1	W_p^2/b	$\sigma^2+b\theta_p^2$
Error	$bk-b-p-rk\underset{\sim}{C}_0$	By Subtraction	σ^2
Total	bk-1	$\underset{\sim}{Y}'\underset{\sim}{Y}-G^2/bk$	----

<u>Remark 5.1</u>. The TFB designs developed for model (2.5) are trend-free also if treatment or block effects are random rather than fixed. Theorem 3.1 holds for random or mixed effects models since condition (3.12) does not depend on distributional assumptions on $\underset{\sim}{Y}$. Expected mean squares in Table 1 would require minor reexpression for a model with random treatment or block effects. When block effects are random and treatment effects are fixed, treatment comparisons may still be made and the demonstrated optimality properties of TFB designs apply.

6. <u>Examples</u>. Given an incidence matrix for a block design and a polynomial trend, a TFB design may or may not exist. Existence theorems and design construction will be discussed in a subsequent paper. Two examples are given below, one a TF_2CB design and one a TF_1BIB design. In the arrays below, letters represent treatments and rows represent blocks. Orthogonal trend components, without normalization, are given in the upper rows of the arrays.

<u>Example 1</u>: A TF_2CB design, $v = 7$, $b = 4$, $p = 2$:

-7	-5	-3	-1	1	3	5	7
7	1	-3	-5	-5	-3	1	7
A	B	C	D	E	F	G	H
G	H	B	A	C	D	F	E
F	E	H	G	B	A	D	C
D	C	E	F	H	G	A	B

<u>Example 2</u>: A TF_1BIB design, $v = 5$, $b = 10$, $k = 3$, $r = 6$, $\lambda = 3$, $p = 1$:

-1	0	1
A	B	C
A	B	D
A	B	E
C	D	A
C	E	A
D	E	A
D	B	C
E	B	C
E	B	D
C	D	E

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20. ABSTRACT

A common polynomial trend in one or more dimensions is assumed to exist over the plots in each block of a classical experimental design. An analysis of covariance model is assumed with trend components represented through use of orthogonal polynomials. The objective is to construct new designs through the assignment of treatments to plots within blocks in such a way that sums of squares for treatments and blocks are calculated as though there were no trend and sums of squares for trend components and error are calculated easily. Such designs are called trend-free and a necessary and sufficient condition for a trend-free design is developed. It is shown that these designs satisfy optimality criteria among the class of connected designs with the same incidence matrix. The analysis of variance for trend-free designs is developed. The paper concludes with two examples of trend-free designs.

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